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Analysis of pressure-volume-temperature relationship for MgO

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Abstract Analysis of pressure-volume-temperature data for MgO has been presented using the ab-initio results obtained by Isaak *et al* Values of compressions at simultaneously elevated pressures and temperatures have been estimated using the volume thermal expansion at $P = 0$ and the ab-initio data An interpolation of the values thus determined yields the results for thermal pressure at high temperatures and high compressions Values of thermal pressures have been used in the formulation of Shanker *et al* to obtain the volume expansions along isobars The results have been found to be in good agreement with the interpolated values based on the first principle calculations

Keywords . Thermal expansivity, equation of state, MgO

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Analysis of pressure-volume-temperature (P-V-T) relationship, *i.e.* equation of state is extremely useful for understanding the thermodynamic and thermoelastic behaviour of solids at high pressure and high temperature [1]. Isaak *et al.* [2] have obtained the P-V-T data for MgO using the potential induced breathing electron gas model which is a type of first principles approach. By this method the Helmholtz energy at constant T is computed as a function of V at selected temperatures. The ab-initio results thus obtained by Isaak *et al* have been found to show very good agreement with measurements of the temperature dependence of several thermoelastic properties [1,3].

In the present study, we analyse the P-V-T data for MgO due to Isaak *et al.* as reported by Anderson in Table 3.1 of Ref. [1] in order to estimate the values of thermal pressure at selected temperatures in the range 300K-2000K and down to a compression of 0.60. These values of thermal pressures are then used to study the temperature dependence of volume along isobars at different pressures with the help of the Shanker equation for thermal expansivity [4].

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The compression values reported by Anderson [Table 3.1 of Ref. 1] are in fact, the values of $V(T, P)/V(T, O)$. These values can be transformed to $V(T, P)/V(T_0, O)$ using the following relationship [5]

$$\eta = \begin{matrix} V(T,P) & V(T,P) & V(T,O) \\ V(T_0,O) & V(T,O) & V(T_0,O) \end{matrix} \tag{1}$$

Here $T_0 = 300$K, the initial temperature. Values of $V(T, O)/V(T_0, O)$ are determined from the data on temperature dependence of density at $P = 0$ [1]. The value at 2000K is determined using the thermal expansivity equation [4] taking the extrapolated value of thermal pressure equal to 10.4 GPa.

Values of η determined from eq. (1) are reported in the form of plots in Figure 1. They represent the isothermal variations of η *versus* P at selected temperatures. For determining the

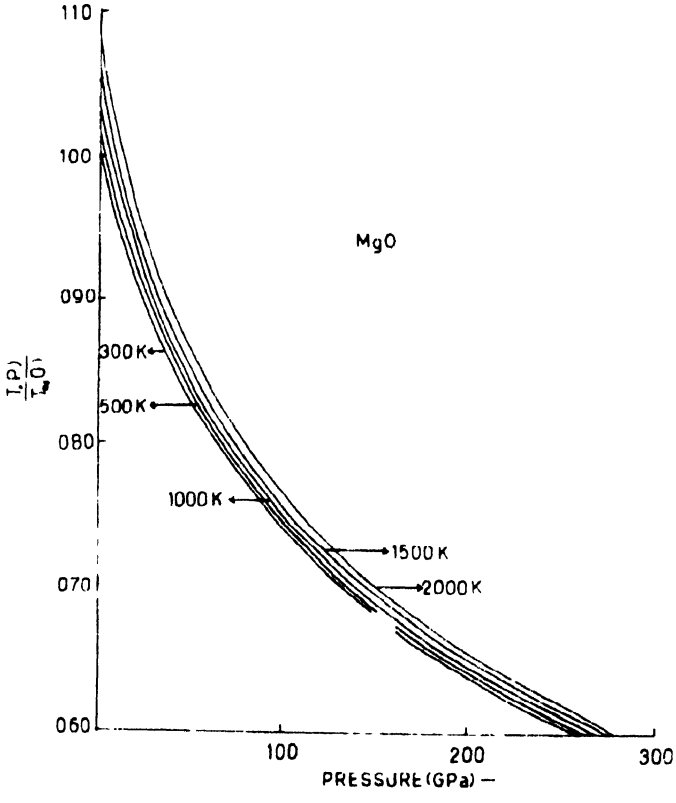

Figure 1 Equation-of-state isotherms for MgO

values of thermal pressures we need the isochoric variations of pressure with temperature. Values of P(T) along isochores are determined from Figure 1 using the interpolation method (Table 1). Values given in Table 1 satisfy the following equation of state

$$P(V, T) = P(V, T_0) + \Delta P_{th}, \tag{2}$$

where

$$\Delta P_{th} = P_{th}(T) - P_{th}(T_0). \tag{3}$$

Table 1. Values of pressure at different temperatures for MgO along isochores corresponding to different values of $\eta = V(T, P)/V(T_0, O)$ Values given in parantheses are $\Delta P_{th} = P_{th}(T) - P_{th}(T_0)$ $T_0 = 300K$

η	Pressures (GPa)				
	300K	500K	1000K	1500K	2000K
1.00	0	1 5	5 0	8 2	11 5
		(1 5)	(5 0)	(8 2)	(11 5)
0 95	10.3	11 8	15 3	18 5	22 0
		(1 5)	(5 0)	(8 2)	(11 7)
0 90	24	25 5	29 0	32 5	36 0
		(1 5)	(5 0)	(8 5)	(12 0)
0 85	41	42 5	46 0	50	54
		(1 5)	(5 0)	(9 0)	(13 0)
0 80	64	66	69	73	78
		(2 0)	(5 0)	(9 0)	(14 0)
0 75	94	96	99	103	109
		(2 0)	(5 0)	(9 0)	(15 0)
0 70	133	135	139	144	150
		(2 0)	(6 0)	(11 0)	(17 0)
0 65	187	189	193	199	205
		(2 0)	(6 0)	(12 0)	(18 0)
0 60	260	263	267	273	278
		(3 0)	(7 0)	(13 0)	(18 0)

Recently, Shanker *et al.* [4] have obtained an equation which can be generalised at any pressure P as follows [6]

$$\frac{V(T,P)}{V(T_0,P)} - 1 = \frac{1 - \left\{1 - 2\left[K'(T_0,P)+1\right]\dfrac{\Delta P_{th}}{K(T_0,P)}\right\}^{1/2}}{\left\{K'(T_0,P)+1\right\}}. \tag{4}$$

where $K(T_0, P)$ is the isothermal bulk modulus at pressure P and $T = T_0$, $K'(T_0, P)$ is the pressure derivative of $K(T_0P)$. We have calculated values of $V(T, P)/V(T_0,P)$ from eq. (4) using ΔP_{th} given in Table 1 and the data on $K(T_0, P)$ and $K'(T_0, P)$ given in Ref. [1]. The values of $V(T, P)/V(T_0,O)$ reported in Table 2 have been determined from eq. (1) and (4).

We have thus presented an analysis of the *P-V-T-* data for MgO based on the *ab-initio* results originally due to Isaak *et al.* [2]. As a result of this analysis, we have determined the values of thermal pressures ΔP_{th} at different temperatures and compressions (Table 1). It is found that ΔP_{th} does not remain constant with η for MgO. This prediction is consistent with recent investigations presented by Anderson [7]. At high compression ($\eta = 0.60$), the value of ΔP_{th} is significantly larger than its value at $\eta = 1$. This is true for the entire range of temperature considered here.

Values of ΔP_{th} determined in the present study have been used in eq. (4) to obtain the values of $V(T, P)$. These values are in close agreement with the interpolated values based on the *ab-initio* results for P-V-T data due to Isaak *et al.* given in Table 2. The reliability of the

Table 2. Values of $\eta = V(T, P)/V(T_0, O)$ for MgO at high pressures and high temperatures calculated from eq. [4] given in column (a), and the interpolated values from Figure 1 based on *ab-initio* data due to Isaak *et al* [2] given in column (b)

P(GPa)	300K	500K		1000K		1500K		2000K	
		(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)
0	1 00	1.009	1.007	1 030	1 028	1 053	1 053	1 081	1 081
10 3	0 95	0 956	0 956	0.973	0.972	0 989	0.989	1.009	1 008
24	0.90	0 905	0 904	0 917	0 915	0 930	0 930	0 945	0.942
41	0 85	0 854	0 853	0 863	0 864	0 875	0 875	0 887	0 887
64	0 80	0 804	0 804	0 810	0 809	0 818	0 818	0 829	0 830
94	0 75	0 753	0 753	0 758	0 757	0 764	0.762	0 773	0 772
133	0 70	0 702	0 702	0 707	0 707	0 712	0 712	0 720	0 719
187	0 65	0 652	0 652	0 655	0 655	0 660	0 660	0.665	0 665
260	0 60	0 602	0 602	0 604	0 605	0 608	0 609	0 611	0 612

ab-initio data [2] has already been demonstrated by Anderson and coworkers [1,3] through a comparison with the experimental data on thermoelastic properties. We can, therefore, conclude that the results obtained in the present study are consistent with the first principle approach [2] as well as with the experimental values of thermoelastic properties. The temperature dependence of thermal expansivity of solids under pressure is of central importance in determining the thermoelastic properties of solids [8-10].

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